O,O-Diethyl dithiophosphate 298-06-6 | DTXSID6027133

Model Performance

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N	Model	Data	

Weighted KNN model

5-fold CV (5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.95	0.69	0.95	0.65	0.96	0.68	

Model Results

Predicted value: 6.72

Global applicability domain: Inside

Local applicability domain index: 9.50e-01

Confidence level: 7.05e-01

Nearest Neighbors from the Training Set

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Acenaphthene Measured: 6.31 Predicted: 6.67

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Pentachlorobenzene Measured: 6.49 Predicted: 6.59

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1,2-Dichloronaphthalene Measured: 6.89 Predicted: 6.90

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trans-Stilbene Measured: 7.48 Predicted: 6.90

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1,5-Dichloronaphthalene

Measured: 6.65 **Predicted:** 6.90